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# Next generation hard X-ray/soft gamma-ray optic design and implementation

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## ABSTRACT

We discuss necessary improvements and further studies relevant to the design and eventual implementation of an accurately modeled multilayer coated X-ray optic operating in the hard X-ray/soft gamma-ray regime. The process improvements are substantiated through lessons learnt from NuSTAR.

## 1. INTRODUCTION

X-ray optics have been used in astronomy for more than 50 years.[1] The last 20 years – considered by some to be the Golden Age of X-ray astronomy – has seen the launch and operation of several observatories relying on focusing telescopes, including ROSAT (1990-1999),[2] ASCA (1993-2000)[3] , BeppoSAX (1996-2002),[4] XMM-Newton (XMM; 1999-present),[5] the Chandra X-ray Observatory (CXO; 1999-present)[6] and Suzaku (2005-present).[7] Joining these very successful satellites in 2012, NuSTAR is the first mission[8] carrying focusing optics operating at hard X-ray energies above 10 keV. This small explorer class mission has already produced fifty peer-reviewed journal papers,[9] with highlights that include reporting on the unambiguous determination of the spin of the black hole in NGC1365[10] and the asymmetry in core-collapse supernovae.[11] With scientific operations now approved to continue into fiscal year 2016, the list of important results from NuSTAR will continue to grow.

NuSTAR's two focusing optics provide unparalleled sensitivity in the 10−79 keV energy band, as well as matching aforementioned much larger missions in sensitivity below 10 keV. The broadband response from 3−79 keV results from the depth-graded multilayer coatings[12] applied to NuSTAR's highly nested Wolter-I-approximating optics.[13]

While the X-ray optics used by previous observatories rely on total external reflection at grazing incidence angles off of single-layer films (e.g., Au for XMM and Ir for CXO), the NuSTAR optics are multilayer based, relying on constructive interference between individual bilayers (e.g., Pt/C) to efficiently reflect radiation according to Bragg's law.[14] Depth-grading the multilayers, varying the period of the bilayer structure in the coatings, is required to achieve a broad energy bandpass. The use of depth-graded multilayers for NuSTAR required the deposition of several hundred thousand bilayers for each of the two optics, with sub-nanometer precision over periods ranging from 2.5 nm to 13 nm. This number of depositions dwarfs that required for previous missions, where a single-layer coating design was used for all shells, e.g., CXO has a 33 nm reflective Ir coating on all four of its shells and XMM has a 250 nm Au coating on all if its 58×3 shells.

The multilayer coatings for a future hard X-ray/soft gamma-ray mission will introduce a tremendous amount of complexity to the coating process and subsequent determination of the optical response, which in turn places strict requirements on modeling, deposition and characterization of the coatings. NuSTAR expended significant effort describing the optical response, finding lower effective area compared to design due to non-uniformity (i.e., period variation across the substrate surface) and an on average shorter-than-designed period,[15] demonstrating the importance of both pre- and post-characterization.

Proposed hard X-ray/soft gamma-ray telescope concepts call for an even greater number of bilayers to ensure high reflection efficiency, and in turn effective area, up to 600 keV, utilizing periods ranging from 1.5 nm to 25 nm.[16] The challenge of simulating a realistic optic response for these telescope concepts rely heavily on ensuring an accurate rendition of the multilayer and its optical properties as it will appear in the optic implementation. The aim of this paper is to elucidate a number of the greatest challenges to this effort.

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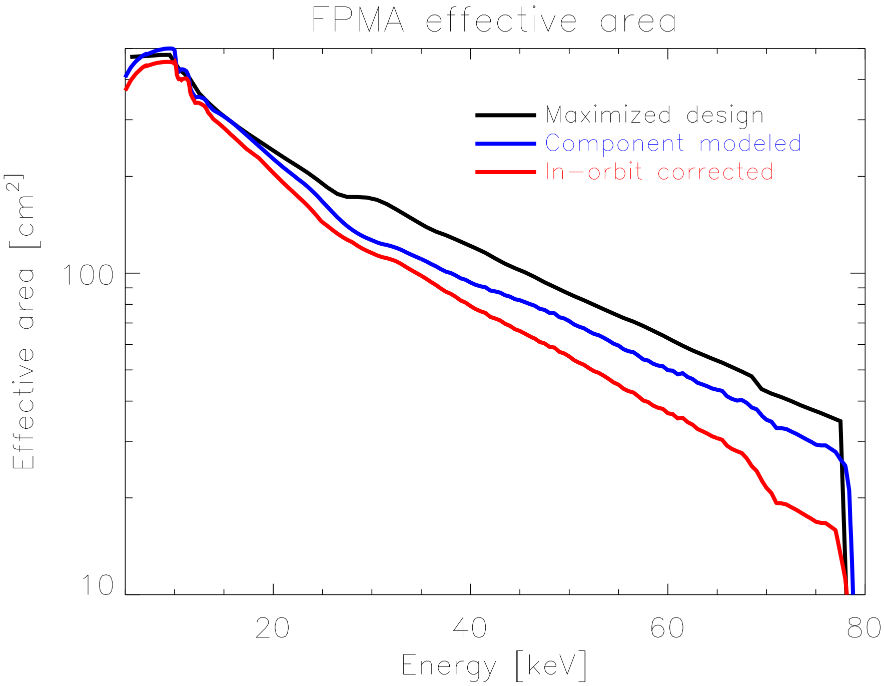


Figure 1. The evolution of the response of an X-ray optic, here illustrated by the NuSTAR focal plane module A (FPMA), is shown. From a maximized design, including ideally uniform multilayers and perfectly smooth substrates (black), to modeling of the figure error and multilayer coating of each individual substrate (blue) and ending in an in-orbit corrected response.

## 2. EMPIRICAL CORRECTIONS TO OPTIC RESPONSE

Previous X-ray focusing missions have found that extensive work[15,17–20] is required to obtain an accurate optic response model. As a result of these efforts, empirical corrections are currently in use for XMM, CXO and NuSTAR. For the total external reflection based optics (XMM and CXO), the corrections account for surface contamination, reflectivity losses due to scattering and decreased material density of the thin film layers as compared to bulk densities. The corrections were established through detailed analysis of on-ground calibration data, combined with observations made in-flight. While a detailed on-ground calibration of NuSTAR was carried out,[21–24] the data are in fact not used to model the in-flight optic response. Instead, the multilayer coating applied to each of the 2376 glass substrate that comprise a single NuSTAR optic, is modelled individually using specular reflectivity data from witness samples on flat Si wafer substrates and an empirical model of the non-uniformity arising from depositing on curved substrates.[15] The resulting 2376 individual multilayers are then ray-traced in an accurate physical representation of a NuSTAR telescope (e.g., the model accounts for obscuration from support structure and the figure error of the mounted mirrors) to form the basis of the in-flight optic response. A final adjustment to the overall effective area, based on observations of the Crab, is also applied.[8,17] The evolution of the effective area through these three stages (maximized design, component modeling and in-orbit correction) is shown in Figure 1. The reduction from design to component model is primarily due to including the non-uniformity of the multilayer and the substrate figure error, while the in-orbit correction likely accounts for second order effects of the non-uniformity.

## 3. CHALLENGES

The growing interest in working at harder X-ray energies and obtaining large collecting areas will drive even more complex multilayer designs and increase the requirement on higher fidelity modeling. While it is unlikely that future missions will ever be able to avoid the use of empirical adjustments to the telescope response, the goal should always be to minimize their use, by controlling the largest sources of modeling uncertainty. The following discussion exemplify what steps are involved in this using lessons learned from the NuSTAR multilayer coatings and response modeling.

### 3.1 From concept to design

Taking a telescope concept to the design level requires the inclusion of implementation-dependent details, e.g., non-uniformities in coatings. Omitting these deviations will make it difficult to obtain accurate estimates for the effective area (Figure 1) and the point spread function of the proposed telescope. Here we focus on the effective area.

Fabrication details become particularly important for the complex multilayer telescopes required for X-ray astronomy. Despite the designs often being termed optimal, the goal of the optimization has usually been to maximize the reflectivity response.[12,16,25–27] While these procedures result in the best *idealized* performance, in practice the designs may be extremely hard to implement. Not least if a number of crucial production conditions are omitted in the design phase. Examples of these effects include: (i) deviations from the prescribed multilayer coating periods laterally along the substrate surface, i.e. the non-uniformity discussed above; (ii) deviations from the prescribed depth-graded periods; (iii) production cycle variations (i.e. run-to-run variations) in multilayer periods. Item (iii) becomes particularly important in a telescope build that includes several thousand optical elements fabricated over several months to years, as passing of time can exacerbate items (i) and (ii).

As such, the multilayer optic optimization "parameter box" should include the notion of ensuring that the deposited coatings follow the intended design as closely as possible and do so even in a production setting. Careful considerations of pre- and post-characterization of the multilayer optic components should be carried out to establish the required steps to ensure a well-understood optic response. For the pre-characterization effort, this would involve understanding the expected design deviations and related requirements prior to flight multilayer deposition, while post-characterization relates to everything from single multilayer reflectivity studies to full end-to-end optic calibration. Figure 1 illustrates that a component-based modeling effort may not be sufficient.

These points depend heavily on the details of the optic implementation and could have a significant impact on everything from mission mass constraints to calibration requirements and, through this, the scientific potential of the mission itself. A fairly straightforward example of this would be that depositing thousands of uniform multilayers on curved substrates may be deemed unfeasible through pre-characterization efforts. This would necessitate coating flat substrates and bending them into the desired shape or relenting on the uniformity requirements. The impact of not controlling the uniformity is apparent from Figure 1 where, to first order, an inaccurate rendition of the multilayer, primarily deriving from non-uniformities, results in a 20% loss in effective area at 50 keV, and, including second order effects, may account for close to a 40% reduction.

### 3.2 New studies

Recent experiments have demonstrated that multilayer response approaching the MeV range continues to behave in accordance with classical wave physics,[28,29] and as such can be modelled using the Fresnel equations when including Névot-Croce factors to account for interface imperfections. However, uncertainties remain which may significantly impact the performance of a full-scale hard X-ray/soft gamma-ray optic.

One of these uncertainties relates to the optical properties (complex index of refraction) of the multilayer constituent materials. These properties are derived from tabulated values of the atomic scattering factor.[30] While studies have shown the tabulated values to be adequate up to 645 keV, the specular reflectivity measurements carried out cannot reveal if a significant (above several percent) error in the absolute reflectivity is present. This is primarily due to the absolute reflectivity also being heavily dependent on interface roughness, material inter-diffusion at the layer interface and other multilayer parameters at a comparable level. XMM, CXO and NuSTAR have all found that more accurate refractive index values were required for their optics,[17,31,32] particularly around the M and L absorption edges, where the independent-atom approximation used in the derivation of tabulated refractive index values break down.[33,34] Measurements of the optical properties increase in difficulty at higher photon energy as the experimental requirements become ever more stringent.

Other structural multilayer parameters must also be studied for a hard X-ray/soft gamma-ray mission. As an example, for a mission operating from below 50 keV to above 500 keV, the micro-roughness governing the specular and non-specular scattering components is unlikely to allow for a single, uniform value to be assumed for all interfaces in the multilayer, irrespective of energy, such as was done for NuSTAR. Implementations of existing formalisms (e.g.,[35, 36]) may be sufficient, but the authors are not aware of any studies having successfully done this in the energy range of interest.

Additional examples of required multilayer studies for a hard X-ray/soft gamma-ray optic includes the physics of continuous layer formation at periods less than 2 nm for the constituent materials, as well as establishing methods of characterizing the coatings accurately using accessible photon energy sources (e.g. 8 keV Cu-$K_\alpha$).

## 4. SUMMARY

Based on experience gained from NuSTAR, we looked at a selection of the challenges associated with the design, fabrication and response modeling of a hard X-ray/soft gamma-ray multilayer optic. Extrapolating these lessons to higher energies, it is clear that process improvements are required with respect to the design and characterization of the multilayer to reduce the need for empirical corrections. In addition to this, more in-depth experimental knowledge and theoretical understanding of the optical properties and response of the multilayers is required to ensure a more accurate optic response model. A number of studies necessary to assist with this were outlined.


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